

4p

Reprinted without change of pagination from  
Journal of Gas Chromatography, ~~pp. 17-20~~, May 1963

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p 17-20

NASA CR-510063 ~~NR~~

**NBS 21123**

Code none

(NASA Contract NAS7-100)  
(NASA CR-51006; JPL-TR-32-449) *reprint*

Reprint

Technical Report No. 32-449

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Chromatography Retention Data**

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This paper presents results of one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under Contract No. NAS 7-100, sponsored by the National Aeronautics and Space Administration.

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PASADENA, CALIFORNIA

May 1963

# FORTTRAN Source Program for Reduction of Gas-Liquid Chromatography Retention Data\*

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Reprinted from JOURNAL OF GAS CHROMATOGRAPHY

Modern high-speed computers are capable of assisting in the reduction and storage of data obtained from gas-liquid partition chromatography (GLPC) measurements. In the past, in order that a computer could be used, it was necessary to prepare machine language programs. This difficulty can now be largely avoided by the application of FORTRAN programming (1), since by this technique the computer is used to aid in the preparation of the program. To illustrate this approach, a typical set of experimental GLPC data for a homologous series of alcohols is reduced by a FORTRAN program developed at this laboratory. The program is designed to give values for the specific retention volumes, the partition coefficients, and the number of theoretical plates

for each peak appearing on a chromatogram. In the course of the data reduction other parameters of importance to the interpretation of results from GLPC measurements are also obtained.

The reduction of GLPC data by FORTRAN is a two step process. The first step requires the preparation of a series of FORTRAN statements that define the mathematical operations by which the GLPC data are to be analyzed; this constitutes the source program. A FORTRAN Compiler translates the source program by means of punched cards into the object program, which is a set of elementary instructions that the computer can understand. The object program is placed into the memory of the computer. The second step is to place the experimental measurements taken from the chromatogram on punched data cards, upon which the computer carries out the designated mathematical operations. The computer presents the reduced data on either IBM cards or as a typed output. Further details for the preparation of the FORTRAN statements are adequately documented elsewhere (2).

Table I gives the source program and symbolism used for the reduction of the GLPC data. This program is intended to be used with an IBM 1620 Data Reduction System, a 1622 Reader Punch, and a 1620 FORTRAN Format Compiler†. Although, it can be modified for use with other equally suitable data reduction systems. The program represents in FORTRAN language the mathematical expressions recommended by the ASTM Committee D-2 on Petroleum Products and Lubricants (3) for the calculation of the corrected retention volume ( $V_R^\circ$ ), the specific retention volume ( $V_g$ ) measured at column temperature and ambient pressures, and the number of theoretical plates. The program also contains expressions for the corrected retention volume  $V_g$  of Littlewood (4); the specific retention volumes measured at either column temperature ( $V_g^{760}$ ) or  $0^\circ\text{C}$  ( $V_g^{760}$ ) but corrected to standard pressure; the partition coefficient  $K_{760}$ , measured at column temperature and corrected to standard pressure; and the pressure correction factor ( $f$ ) of James and Martin (5).

\*This paper presents the results of one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under Contract No. NAS 7-100, sponsored by the National Aeronautics and Space Administration.

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\*Computermat, Inc. 1111 Wilshire Blvd., Los Angeles 17, California.

Table I. Source Program and Symbolism for GLPC Data Reduction

### A. Source Program

```

1. Format (15X, 40HGAS Liquid Chromatography Retention Data)
2. Format (/10X, 2HFU, 12X, 3HPIG, 11X, 1HP, 13X, 1HT, 13X, 1HZ)
3. Format (10X, 3HSWT, 11X, 5HRTAIR, 9X, 1HD, 13X, 2HTC, 12X, 1HN)
4. Format (10X, 4HFSTP, 10X, 2HPT, 12X, 2HPI, 12X, 2HPR, 12X, 2HPF)
5. Format (10X, 4HPGCF, 10X, 2HVP, 12X, 2HTR)
6. Format (10X, 2HRT, 12X, 1HW, 13X, 4HVG7, 10X, 3HVDRO, 11X, 3HVG7)
7. Format (10X, 3HCRT, 11X, 2HTP, 12X, 3HVG7, 11X, 3HCAY, 11X, 2HVG/)
8. Format (9F6.0, 12)
9. Format (5F14.4)
19. Format (4F14.4, 9X, 13)
10. Format (5F14.3)
20. Format (3F14.3)
11. Format (F6.0, F6.0, F6.0, F6.0, F6.0, F6.0, F6.0, F6.0)
12. Format (5F14.3/5F14.3/)
    If (Sense Switch 3) 30, 31
30. Print 1
31. Punch 1
    DO 90 I=1, 100
    Read 8, FU, PIG, P, T, Z, SWT, RTAIR, D, TC, N
    If (Sense Switch 3) 32, 33
32. Print 2
33. Punch 2
    If (Sense Switch 3) 34, 35
34. Print 9, FU, PIG, P, T, Z
35. Punch 9, FU, PIG, P, T, Z
    If (Sense Switch 3) 36, 37
36. Print 3
37. Punch 3
    If (Sense Switch 3) 64, 65
64. Print 19, SWT, RTAIR, D, TC, N
65. Punch 19, SWT, RTAIR, D, TC, N
    VP=EXP (2.302585*(8.10765-(1750.286/(235.0+T))))
    FSTP=(FU*(P-VP)*273.1)/((T+273.1)*760.)

```

```

PT=(P*14.696)/760.
PI=((PIG+PT)*760.)/14.696
PR=PI/P
PF=PR**2-1.
PGCF=1.5*PF/(PR**3-1.)
TR=1.0E4/(TC+273.1)
If (Sense Switch 3) 38, 39
38. Print 4
39. Punch 4
    If (Sense Switch 3) 42, 43
42. Print 10, FSTP, PT, PI, PR, PF
43. Punch 10, FSTP, PT, PI, PR, PF
    If (Sense Switch 3) 40, 41
40. Print 5
41. Punch 5
    If (Sense Switch 3) 66, 67
66. Print 20, PGCF, VP, TR
67. Punch 20, PGCF, VP, TR
    If (Sense Switch 3) 44, 45
44. Print 6
45. Punch 6
    If (Sense Switch 3) 46, 47
46. Print 7
47. Punch 7
    Dimension CM(100), X(100)
    K=1
21. Read 11, CM(K), X(K), CM(K+1), X(K+1), CM(K+2), X(K+2), CM(K+3), X(K+3)
    K=K+4
    If (K-N) 21, 21, 22
22. DO 80 J=1, N
    RTN=RTAIR/Z
    RT=CM(J)/Z
    CRT=RT-RTN
    W=X(J)/Z
    FPP=(FU*CRT/SWT)*((P-VP)/)*PGCF
    VRO=FU*PGCF*((P-VP)/P)*((TC+273.1)/(T+273.1))*CRT
    VG=FPP*273.1/(T+273.1)
    VG7=VG*P/760.
    VGP=FPP*(TC+273.1)/(T+273.1)
    VGP7=VGP*P/760.
    CAY=(VG7*(TC+273.1)*D)/273.1
    TP=16.*((RT/W)**2)
    If (Sense Switch 3) 48, 49

```

```

48. Print 12, RT, W, VGP7, VRO, VG7, CRT, TP, VGP, CAY, VG
49. Punch 12, RT, W, VGP7, VRO, VG7, CRT, TP, VGP, CAY, VG
80. Continue
90. Continue
End

```

### B. FORTRAN Source Program Measurements

FU Flow measured with a soap bubble meter (ml per min).  
 PIG Pressure inlet gauge (lb per sq. in.).  
 P Barometric pressure (mm of mercury).  
 T Temperature at which gas flow measured (°C).  
 Z Chart units per min (may be centimeters or inches as long as consistent units for retention time and peak widths are used).  
 SWT Weight of liquid phase in column (grams).  
 RTAIR Retention time of air in same units as Z.  
 D Density of liquid phase at column temperature (grams per ml).  
 TC Column temperature (°C).  
 N Number of peaks in the chromatogram which are computed.  
 CM Retention distance on chart in units which are consistent with Z.  
 X Peak width in units consistent with Z.

### C. Column Parameters from Reduction of Data

FSTP Flow reduced to standard temperature and pressure (ml per min).  
 PT Atmospheric pressure (lb per square in.).  
 PI Inlet pressure (mm of mercury).  
 PR Ratio of inlet to outlet pressures.  
 PF Pressure factor.  
 PGCF Pressure gradient correction factor.  
 VP Vapor pressure of water at temperature T ((mm of mercury).  
 RT Reciprocal of absolute column temperature times ten thousand.

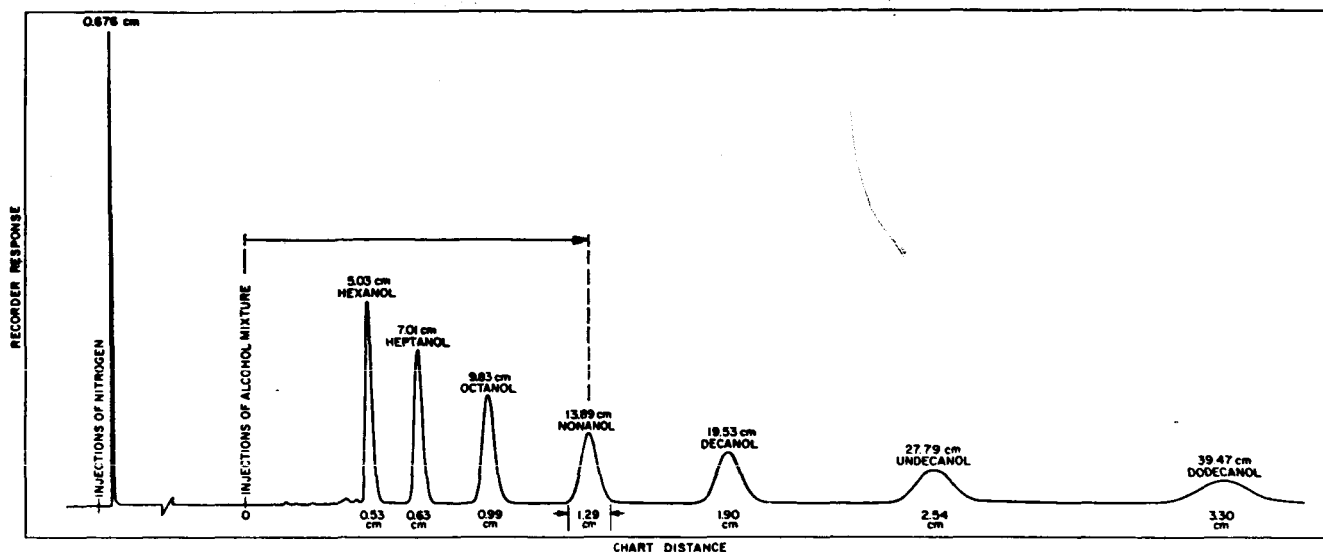


Figure 1. Chromatography chart.

The conditions for the above separation were: the column was 6 ft. in length with 25% wt/wt of Carbowax 20M on a Chromosorb P 30/60 mesh solid support. The total weight of liquid phase was 4.40g. The helium carrier gas flow of 65.22 ml/min was measured at 21.0° C and 729.0 mm. The column temperature and inlet pressure were 191.1° C and 10.60 lb/in.<sup>2</sup> gauge, respectively. The recorder chart speed was 2.00 cm/min, and the density of the liquid phase at 191.1° C is 1.070 g/ml (6). The proper organization of the above measurements is shown below.

6	12	18	24	30	36	42	48	54	60
6.5, .2, 2.	1.0, .6, 0.	7.2, 9, .0.	2.1, .0.	2, .0, 0.	4, .4, 0.	0, .6, 7, 6.	1, .0, 7, 0.	1, 9, 1, .1.	0, 7
5, .0, 3.	0, .5, 3.	7, .0, 1.	0, .6, 3.	9, .8, 3.	0, .9, 9.	1, 3, .8, 9.	1, .2, 9.		
1, 9, .5, 3.	1, .9, 0.	2, 7, .7, 9.	2, .5, 4.	3, 9, .4, 7.	3, .3, 0.	0, .0.	0, .0.		

Data for test case.

#### D. Reduced Data for Components on Chromatogram

- RT Retention time of component (min).
- W Peak width of component (min).
- CRT Corrected retention time (min).
- TP Theoretical plates.
- CAY Partition coefficient.
- VRO Corrected retention volume (ml).
- VG Specific retention volume at zero degrees centigrade but not to standard pressure (ml per gram).
- VG7 Specific retention volume at standard temperature and pressure (ml per gram).
- VGP Specific retention volume at column temperature and at ambient pressure (ml per gram).

VGP7 Specific retention volume at temperature corrected to standard pressure (ml per gram).

The data cards should be punched with nine fields of six columns each with one field of two columns at the end. The column input measurements are read by the computer in the following order: FU, FIG, P, T, Z, SWT, RTAIR, D, TC, and N. The first nine fields are floating point numbers with N being a fixed point number. If N is less than ten it must have a zero to fill the field. The input measurements for the components are read as eight fields of six columns each with four pairs of retention distances and peak widths per data card. Any fields not used must be completed with float-

ing point zeros. In some instances it may not be practical to measure peak width. In these cases the best procedure is to repeat the value for the retention distance as the peak width and this leads to the number 16 which appears as a fictitious number of theoretical plates.

Figure 1 shows a chromatogram for a series of homologically related alcohols, and presents the proper organization of the input measurements for placement onto a data card for setting up the program. In Table II the computed data for the homologous series of alcohols is given so that it may be used as a check case. The time required to compute the check chromatogram is about 35 seconds.

To make the program economical of computer time there is a provision which allows the computed data to be punched on IBM cards. This is

Table II. Gas Liquid Chromatography Retention Data

	FU	FIG	P	T	Z
	65.2200	10.60000	729.0000	21.0000	2.0000
	SWT	RTAIR	D	TC	N
	4.4000	.6760	1.0700	191.1000	7
	FSTP	PT	PI	PR	PF
	56.606	14.096	1277.176	1.751	2.069
	PGCF	VP	TR		
	.709	18.646	21.542		
	RT	W	VGP7	VRO	VG7
	CRT	TP	VGP	CAY	VG
(HEXANOL)	2.515	.265	33.757	154.849	19.860
	2.177	1441.133	35.192	36.120	20.704
(HEPTANOL)	3.505	.315	49.108	225.267	28.891
	3.167	1980.956	51.197	52.546	30.120
(OCTANOL)	4.915	.495	70.972	325.560	41.755
	4.577	1577.453	73.990	75.940	43.530
(NONANOL)	6.945	.645	102.450	469.953	60.274
	6.607	1855.004	106.807	109.622	62.837
(DECANOL)	9.765	.950	146.179	670.538	86.000
	9.427	1690.508	152.395	156.411	89.657
(UNDECANOL)	13.895	1.270	210.220	964.303	123.677
	13.557	1915.268	219.159	224.935	128.937
(DODECANOL)	19.735	1.650	300.777	1379.700	176.954
	19.397	2288.897	313.568	321.832	184.479

controlled by sense switch 3 on the 1620 console. By having sense switch 3 in the *on* position, both typewriter and punch card output of data results. This mode is slow, but allows checking at the start of the run. When sense switch 3 is in the *off* position, only card punching will occur. In the event that any errors occur during computing they will be noted on the typewriter. The output data can be edited by dropping in punched title cards at appropriate points in the deck of cards before printing on an IBM 407 accounting machine. The data output cards can also be used as input cards for other programs or may be stored as such. It is strongly recommended that care and attention to detail be given to the preparation of the punched cards. The lack of a decimal point or failure to fill in unused fields with zeros will lead to difficulties.

The program has been processed

on two separate IBM 1620 systems at the Jet Propulsion Laboratory and an independent check was run by Computermat, Inc.\* using the source program and data presented in this paper. ■

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Manuscript received April 12, 1963.